

## *In Vitro* Data for Substances Tested in the ICE Test Method: Sorted by Reference

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	<i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	Overall <i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	<i>In Vitro</i> Classif. (EPA) <sup>3,4</sup>	Overall <i>In Vitro</i> Classif. (EPA)	<i>In Vitro</i> Classif. (EU) <sup>5,6</sup>	Overall <i>In Vitro</i> Classif. (EU)	Reference
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	1	1.4	0.4	9.6	2B	2A	III	II	NI	R36	Balls et al. (1995)
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	2	1	1.7	49	2A		II		R36		Balls et al. (1995)
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	3	1.83	1.17	7.64	2B		III		R36		Balls et al. (1995)
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	4	3	1	13.8	2A		II		R36		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.9%	Aldrich	1	1.2	0.9	6.7	2B	2B	III	III	NI	NI	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.9%	Aldrich	2	2	1.3	42	2A		II		R36		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.9%	Aldrich	3	1.33	1.5	12.33	2B		III		NI		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.9%	Aldrich	4	2	0.5	6	2B		III		NI		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	1	1	0.7	3.2	2B	2A	III	II	NI	R36	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	2	2	2	56	2A		II		R36		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	3	1.83	1.67	14.67	2A		II		R36		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	4	2	1	10	2B		III		R36		Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	1	1.8	0.6	18	2A/2B	2A	II/III	II	R36	R36	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	2	1.3	2.3	47	2A		II		R36		Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	3	2.67	1.5	12.66	2A		II		R36		Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	4	2	3	8.8	2A		II		R36		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	1	3	3	37.7	1	1	I	I	R41	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	2	3	2.3	95	1		I		R41		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	3	3	2.33	40.72	1		I		R41		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	4	3	2	41.1	1		I		R41		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	1	3	2.6	36.3	1	1	I	II	R41	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	2	1	2	42	2A		II		R36		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	3	3	2	33.77	1		I		R41		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	4	3	3	68.9	1		I		R41		Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	1	1.8	1.8	13.9	2A	2A	II	II	R36	R36	Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	2	0.5	2.7	42	1		I		R41		Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	3	1	2	14.67	2A/2B		II/III		R36		Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	4	1	2	32.2	2A		II		R36		Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	1	2.6	1.4	15.8	2A	2A	II	II	R36	R36	Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	2	1.3	2	47	2A		II		R36		Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	3	1.67	1.5	13.1	2A/2B		II/III		R36		Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	4	1	2	13	2A/2B		II/III		R36		Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	1	0	0.4	1.7	NI	2B	IV	III	NI	NI	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	2	0.2	1	27	2B		III		NI/R36		Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	3	0	1.33	19.17	2B		III		NI		Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	4	1	1	20	2B		III		R36		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	1	1	0.5	5.4	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	2	1.3	3	89	1		I		R41		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	3	0.67	0.5	-1.4	NI		IV		NI		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	4	2	1	12.7	2A/2B		II/III		R36		Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	Sf	0.1%	98%	Sigma	1	1	0	2.2	NI	2B	IV	III	NI	NI/R36	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	Sf	0.1%	98%	Sigma	2	0.7	0	21	2B		III		NI		Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	Sf	0.1%	98%	Sigma	3	0.67	1	10.29	2B		III		NI		Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	Sf	0.1%	98%	Sigma	4	1	1	14.6	2B		III		NI/R36		Balls et al. (1995)

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Cetylpyridinium bromide (10%)	140-72-7	liquid	Sf	10%	98%	Sigma	1	2.6	1	25.8	2A	2A	II	R36	R36	Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	Sf	10%	98%	Sigma	2	1.7	2	41	2A		II	R36		Balls et al. (1995)	
(Cetyl)pyridinium bromide (10%)	140-72-7	liquid	Sf	10%	98%	Sigma	3	2	1.67	27.2	2A	2A	II	R36		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	Sf	10%	98%	Sigma	4	3	3	17.8	1		I	R41		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	Sf	6%	98%	Sigma	1	2	1.2	27.2	2A	2A	II	R36	R36	Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	Sf	6%	98%	Sigma	2	2	0.5	49	2A		II	R36		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	Sf	6%	98%	Sigma	3	3	1.83	24.55	2A		II	R36		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	Sf	6%	98%	Sigma	4	2.7	1.7	13.5	2A		II	R36		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	1	3	4	32	1	1	I	R41	R41	Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	2	3	4	150	1		I	R41		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	3	3	3	53.13	1		I	R41		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	4	3	4	-	1		I	R41		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	1	2.2	2.2	24.7	2A	1	II	R36	R41	Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	2	3	2	103	1		I	R41		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	3	3	2.5	35.74	1		I	R41		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	4	3	2.5	45.3	1		I	R41		Balls et al. (1995)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	1	2.8	3	12.8	1	1	I	R41	R41	Balls et al. (1995)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	2	1	2.7	75	1		I	R41		Balls et al. (1995)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	3	2	1.5	6.36	2B		III	R36		Balls et al. (1995)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	4	1	2	6.7	2B		III	R36		Balls et al. (1995)	
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	1	2.6	2	12.2	2A	2A/2B	II	R36	R36	Balls et al. (1995)	
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	2	1	0	22	2B		III	R36		Balls et al. (1995)	
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	3	2	1.5	17.07	2A/2B		II/III	R36		Balls et al. (1995)	
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	4	2	2	40.9	1		I	R36		Balls et al. (1995)	
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	1	2.3	0.8	12.7	2A/2B	2A	II/III	R36	R36	Balls et al. (1995)	
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	2	2	1.3	26	2A		II	R36		Balls et al. (1995)	
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	3	1.83	1.67	17.15	2A		II	R36		Balls et al. (1995)	
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	4	1.8	0.8	16.8	2A/2B		II/III	R36		Balls et al. (1995)	
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	1	3	2.4	43.8	1	1	I	R41	R41	Balls et al. (1995)	
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	2	3	2.7	74	1		I	R41		Balls et al. (1995)	
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	3	3	2.5	35.9	1		I	R41		Balls et al. (1995)	
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	4	3	3	62.7	1		I	R41		Balls et al. (1995)	
2,5-Dimethylohexanediol	110-03-2	solid	I	neat	99.5%	BASF	1	2	1	11.9	2B	2B	III	R36	R36	Balls et al. (1995)	
2,5-Dimethylohexanediol	110-03-2	solid	I	neat	99.5%	BASF	2	3	3	64	1		I	R41		Balls et al. (1995)	
2,5-Dimethylohexanediol	110-03-2	solid	I	neat	99.5%	BASF	3	1.33	1.67	11.57	2B		III	R36		Balls et al. (1995)	
2,5-Dimethylohexanediol	110-03-2	solid	I	neat	99.5%	BASF	4	2	1	6.7	2B		III	R36		Balls et al. (1995)	
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	1	2.8	2.8	30.7	1	1	I	R41	R41	Balls et al. (1995)	
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	2	2	3	74	1		I	R41		Balls et al. (1995)	
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	3	2.5	2.33	35.88	2A		II	R36		Balls et al. (1995)	
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	4	2	2.3	34.6	2A		II	R36		Balls et al. (1995)	
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	1	2	2	22	2A	2A	II	R36	R36	Balls et al. (1995)	
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	2	1.7	2.3	76	2A		II	R36		Balls et al. (1995)	
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	3	2	2	25.08	2A		II	R36		Balls et al. (1995)	
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	4	3	2	23	2A		II	R36		Balls et al. (1995)	

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2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	1	2	2.2	43	2A	2A	II	R36	R36	Balls et al. (1995)	
2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	2	1	2.3	62	2A		II	R36		Balls et al. (1995)	
2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	3	3	1.5	13.31	2A		II	R36		Balls et al. (1995)	
2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	4	1	2	52.4	2A		II	R36		Balls et al. (1995)	
Ethyl 2-methylacetooacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	1	0.4	0.3	-2.8	NI	2B	IV	NI	NI	Balls et al. (1995)	
Ethyl 2-methylacetooacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	2	1	0	7	2B		III	NI		Balls et al. (1995)	
Ethyl 2-methylacetooacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	3	0.67	1	11.52	2B		III	NI		Balls et al. (1995)	
Ethyl 2-methylacetooacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	4	1	0.5	4.5	NI		IV	NI		Balls et al. (1995)	
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	1	1.2	0.4	7.2	2B	2B	III	NI	NI	Balls et al. (1995)	
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	2	2	2	31	2A		II	R36		Balls et al. (1995)	
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	3	0	0	1.44	NI		IV	NI		Balls et al. (1995)	
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	4	1	0.5	6.7	2B		III	NI		Balls et al. (1995)	
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	1	0.9	1.2	5.3	2B	2B	III	NI	NI	Balls et al. (1995)	
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	2	0	0.2	11	NI		IV	NI		Balls et al. (1995)	
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	3	1	0.5	2.82	NI		IV	NI		Balls et al. (1995)	
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	4	1	1	4.3	2B		III	NI		Balls et al. (1995)	
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	1	1.2	1	5	2B	2B	III	NI	NI	Balls et al. (1995)	
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	2	0	0	11	NI		IV	NI		Balls et al. (1995)	
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	3	1.17	1	8.3	2B		III	NI		Balls et al. (1995)	
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	4	2	0.5	29.4	2A		II	R36		Balls et al. (1995)	
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	1	2.8	1.6	17.4	2A	1	II	R36	R41	Balls et al. (1995)	
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	2	0.2	1.7	82	2A		II	R36		Balls et al. (1995)	
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	3	3	2.83	28.89	1		I	R41		Balls et al. (1995)	
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	4	3	3	58.9	1		I	R41		Balls et al. (1995)	
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	1	3	4	40.3	1	1	I	R41	R41	Balls et al. (1995)	
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	2	3	3	224	1		I	R41		Balls et al. (1995)	
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	3	3	2.5	36.96	1		I	R41		Balls et al. (1995)	
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	4	3	3	97.8	1		I	R41		Balls et al. (1995)	
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	1	2.8	2.5	46.4	1	1	I	R41	R41	Balls et al. (1995)	
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	2	3	2.7	93	1		I	R41		Balls et al. (1995)	
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	3	3	2.5	37.06	1		I	R41		Balls et al. (1995)	
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	4	3	2	69.2	1		I	R41		Balls et al. (1995)	
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	1	2	1.6	23.3	2A	1	II	R36	R41	Balls et al. (1995)	
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	2	0.7	2.7	72	1		I	R41		Balls et al. (1995)	
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	3	3	2.5	37.84	1		I	R41		Balls et al. (1995)	
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	4	2.3	0.5	8.9	2B		III	NI		Balls et al. (1995)	
Maneb	12427-38-2	solid	S	neat	90%	EPA	1	0	0.5	2.8	NI	NI	IV	NI	NI	Balls et al. (1995)	
Maneb	12427-38-2	solid	S	neat	90%	EPA	2	1	2	33	2A		II	R36		Balls et al. (1995)	
Maneb	12427-38-2	solid	S	neat	90%	EPA	3	0	0.5	8.03	NI		IV	NI		Balls et al. (1995)	
Maneb	12427-38-2	solid	S	neat	90%	EPA	4	1	1	6.7	2B		III	NI		Balls et al. (1995)	
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	1	1.4	2.4	20.3	2A	1	II	R36	R41	Balls et al. (1995)	
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	2	1	2.7	93	1		I	R41		Balls et al. (1995)	
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	3	2	2	22.5	2A		II	R36		R41	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	4	3	3	17.5	1		I	R41		R41	Balls et al. (1995)

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Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	<i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	Overall <i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	<i>In Vitro</i> Classif. (EPA) <sup>3,4</sup>	Overall <i>In Vitro</i> Classif. (EPA)	<i>In Vitro</i> Classif. (EU) <sup>5,6</sup>	Overall <i>In Vitro</i> Classif. (EU)	Reference			
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	1	0.4	0.3	4.5	NI	NI	IV	IV	NI	NI	Balls et al. (1995)			
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	2	0.5	0.7	44	2A		II		R36				Balls et al. (1995)	
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	3	0.17	0.5	4.93	NI		IV					NI		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	4	1	1	10.7	2B		III					NI		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	1	0.4	0.5	2.3	NI	NI	IV	IV	NI	NI	Balls et al. (1995)			
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	2	1	0	22	2B		III					NI		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	3	0	0.5	5.83	NI		IV					NI		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	4	1	0.5	0	NI		IV					NI		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	1	2	2.2	23.1	2A	1	II	I	R36	R41	Balls et al. (1995)			
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	2	2.7	3	99	1		I		R41				Balls et al. (1995)	
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	3	3	2.33	34.88	1		I		R41				Balls et al. (1995)	
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	4	3	2	12.6	2A		II		R36				Balls et al. (1995)	
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	1	2.6	2	26.5	2A	2A	II	II	R36	R36	Balls et al. (1995)			
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	2	3	3	64	1		I		R41				Balls et al. (1995)	
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	3	2	2.17	21.69	2A		II		R36				Balls et al. (1995)	
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	4	2	2	12.3	2A		II		R36				Balls et al. (1995)	
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	1	1	0.9	5.6	2B	2B	III	III	NI	R36	Balls et al. (1995)			
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	2	1	1	24	2B		III		R36				Balls et al. (1995)	
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	3	2	1	8.86	2B		III		R36				Balls et al. (1995)	
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	4	1	1	46.7	2A		II		R36				Balls et al. (1995)	
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	1	3	3	46.6	1	1	I	I	R41	R41	Balls et al. (1995)			
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	2	3	2.7	122	1		I		R41				Balls et al. (1995)	
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	3	3	2.5	44.19	1		I		R41				Balls et al. (1995)	
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	4	3	3	64.1	1		I		R41				Balls et al. (1995)	
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	1	2	2.4	36.5	2A	2A	II	II	R36	R36	Balls et al. (1995)			
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	2	1.3	2	108	2A		II		R36				Balls et al. (1995)	
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	3	1.17	1.5	10.18	2B		III		NI				Balls et al. (1995)	
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	4	2	1	25.7	2A		II		R36				Balls et al. (1995)	
Parafluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	1	3	2.2	35.3	1	1	I	I	R41	R41	Balls et al. (1995)			
Parafluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	2	3	2	79	1		I		R41				Balls et al. (1995)	
Parafluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	3	3	2	33.44	1		I		R41				Balls et al. (1995)	
Parafluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	4	3	2	38.5	1		I		R41				Balls et al. (1995)	
Polyethylene glycol 400	25322-68-3	liquid	Sf	undiluted	n.p.	Aldrich	1	1.4	1	9.8	2B	2B	III	III	NI	R36	Balls et al. (1995)			
Polyethylene glycol 400	25322-68-3	liquid	Sf	undiluted	n.p.	Aldrich	2	0.2	0	26	NI		IV					NI		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	Sf	undiluted	n.p.	Aldrich	3	2	1	5.88	2B		III		R36				Balls et al. (1995)	
Polyethylene glycol 400	25322-68-3	liquid	Sf	undiluted	n.p.	Aldrich	4	1	0.5	14.8	2B		III		R36				Balls et al. (1995)	
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	1	1	0.7	8	2B	2B	III	III	NI	R36	Balls et al. (1995)			
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	2	0.2	0	25	2B		III					NI		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	3	1.67	1	10.45	2B		III		R36				Balls et al. (1995)	
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	4	1.3	1.7	25.3	2A		II		R36				Balls et al. (1995)	

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Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	1	2.6	1.6	33	1		1	R41		Balls et al. (1995)		
Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	2	3	3	143	1		1	R41		Balls et al. (1995)		
Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	3	3	2	23.02	2A		1	I	R36	R41	Balls et al. (1995)	
Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	4	2	3	28.6	1/2A		1	I/H	R36/R41		Balls et al. (1995)	
Pyridine	110-86-1	liquid	S	undiluted	>99.9%	Aldrich	1	3	2	32.7	1		1	R41		Balls et al. (1995)		
Pyridine	110-86-1	liquid	S	undiluted	>99.9%	Aldrich	2	3	3	95	1		1	R41		Balls et al. (1995)		
Pyridine	110-86-1	liquid	S	undiluted	>99.9%	Aldrich	3	3	2.5	37.47	1		1	R41		R41	Balls et al. (1995)	
Pyridine	110-86-1	liquid	S	undiluted	>99.9%	Aldrich	4	3	3	78.6	1		1	R41		Balls et al. (1995)		
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	1	1.2	0.6	4.1	2B		2B	III	NI		Balls et al. (1995)	
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	2	0.2	0.2	12	NI		2B	IV	NI		Balls et al. (1995)	
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	3	2	2	11.49	2A		2B	II	R36		Balls et al. (1995)	
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	4	1	0.5	6.8	2B		2B	III	NI		Balls et al. (1995)	
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	1	1	0.6	14.1	2B		2A	III	NR/R36		Balls et al. (1995)	
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	2	0.7	2.3	55	2A		2A	II	R36		Balls et al. (1995)	
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	3	2.33	2.5	30.31	2A		2A	II	R36		Balls et al. (1995)	
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	4	2	2	33.3	2A		2A	II	R36		Balls et al. (1995)	
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG <sup>2</sup>	Fisher	1	3	4	32	1		1	I	R41		Balls et al. (1995)	
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG	Fisher	2	3	3.3	194	1		1	I	R41		R41	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG	Fisher	3	3	3.17	68.86	1		1	I	R41		Balls et al. (1995)	
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG	Fisher	4	3	4	151.7	1		1	I	R41		Balls et al. (1995)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	1	0.6	0.4	7	2B		2B	III	NI		Balls et al. (1995)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	2	1	0.2	33	2A		2B	II	R36		Balls et al. (1995)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	3	1.67	1	9.56	2B		2B	III	R36		Balls et al. (1995)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	4	1	1	12.2	2B		2B	III	NI		Balls et al. (1995)	
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	1	1	0.2	3.9	NI		2B	IV	NI		Balls et al. (1995)	
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	2	0	0	39	2B		2B	III	R36		Balls et al. (1995)	
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	3	1	0	2.75	NI		2B	IV	NI		Balls et al. (1995)	
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	4	1	1	15.9	2B		2B	III	NR/R36		Balls et al. (1995)	
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	1	0.7	0.7	6.3	2B		2B	III	NI		Balls et al. (1995)	
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	2	0.2	0	24	2B		2B	III	NI		Balls et al. (1995)	
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	3	0.5	0.5	2.62	NI		2B	IV	NI		Balls et al. (1995)	
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	4	1	0	2.4	NI		2B	IV	NI		Balls et al. (1995)	
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	1	0.6	0.5	3.1	NI		2B	IV	NI		Balls et al. (1995)	
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	2	0.2	0.7	23	2B		2B	III	NI		Balls et al. (1995)	
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	3	1.33	1	7.54	2B		2B	III	NI		Balls et al. (1995)	
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	4	1	0.5	14.6	2B		2B	III	NI		Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	1	1.3	1	7.5	2B		2B	III	NI		Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	2	1	2	31	2A		2B	II	R36		Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	3	1.5	1.5	7.3	2B		2B	III	NI		Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	4	1	1	8.9	2B		2B	III	NI		Balls et al. (1995)	
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	2	1.4	1	5.2	2B		2A	III	NI		Balls et al. (1995)	
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	3	2	1.3	29	2A		2A	II	R36		Balls et al. (1995)	
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	4	1.33	2	13.87	2A/2B		2A	II/III	R36		Balls et al. (1995)	
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	1	1	2	58.2	2A		2A	II	R36		Balls et al. (1995)	

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Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	2	2.4	1.2	13.2	2A/2B	2A	II/III	R36	R36	Balls et al. (1995)	
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	3	2.3	2	38	2A		II	R36		Balls et al. (1995)	
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	4	1.5	2.5	27.88	2A		II	R36		Balls et al. (1995)	
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	1	1.7	2	26.4	2A		II	R36		Balls et al. (1995)	
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	2	3	4	32	1		I	R41	R41	Balls et al. (1995)	
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	3	3	4	153	1		I	R41		Balls et al. (1995)	
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	4	*	4	*	*		*	*		Balls et al. (1995)	
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	1	3	4	*	1		I	R41		Balls et al. (1995)	
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	2	1.4	0.1	9.9	2B	2A/2B	III	NI	R36	Balls et al. (1995)	
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	3	1	0.8	29	2A/2B		II/III	R36		Balls et al. (1995)	
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	4	2.67	1.17	20.2	2A		II	R36		Balls et al. (1995)	
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	1	1.7	1	11.2	2B		III	R36		Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	2	1	0.6	9.8	2B		III	NI	R36	Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	3	1.3	0	38	2A		II	R36		Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	4	2	0	3.97	2B		III	NI		Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	1	1	2	39.6	2A		II	R36		Balls et al. (1995)	
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	2	1	1	3.6	2B	2B	III	NI	NI	Balls et al. (1995)	
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	3	0.2	0	31	2B		III	NI/R36		Balls et al. (1995)	
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	4	2.5	1	5.63	2B		III	R36		Balls et al. (1995)	
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	1	1	0.5	6.7	2B		III	NI		Balls et al. (1995)	
TNO-01 (Formulation-1) <sup>7</sup>	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-02 (Formulation-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2.7	2	24	2A	2A	II	II	R36	R36	Prinsen (1996)
TNO-03 (Pesticide-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.6	0.3	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-04 (Detergent-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.5	1.5	9	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-05 (Silicone powder-1)	n.p.	solid	I	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-06 (Lubricant)	n.p.	gel	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-07 (Ink-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.8	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-08 (Ink-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.1	0	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-09 (Paint)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.3	0.5	5	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-10 (Silicone powder-2)	n.p.	solid	I	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	solid	n.p.	undiluted	n.p.	n.p.	-	2	1.3	19	2A	2A	II	II	R36	R36	Prinsen (1996)
TNO-12 (Formulation-3)	n.p.	paste	n.p.	undiluted	n.p.	n.p.	-	2.5	2	35	2A	2A	II	II	R36	R36	Prinsen (1996)
TNO-13 (Pesticide-2)	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.7	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-14 (Polydisaccharide)	n.p.	liquid	n.p.	14.5%	n.p.	n.p.	-	0.3	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-15 (Polydisaccharide)	n.p.	liquid	n.p.	50%	n.p.	n.p.	-	0	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-16 (Liquid nylon product)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-17 (Solvent-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.3	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-18 (Solvent-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-19 (Solvent-3)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-20 (Solvent-4)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.5	0.3	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-21 (Solvent-5)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.3	0.3	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-22 (Solvent-6)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0.3	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-23 (Solvent-7)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-24 (Solvent-8)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-25 (Solvent-9)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)

## *In Vitro* Data for Substances Tested in the ICE Test Method: Sorted by Reference

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	<i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	Overall <i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	<i>In Vitro</i> Classif. (EPA) <sup>3,4</sup>	Overall <i>In Vitro</i> Classif. (EPA)	<i>In Vitro</i> Classif. (EU) <sup>5,6</sup>	Overall <i>In Vitro</i> Classif. (EU) <sup>5,6</sup>	Overall <i>In Vitro</i> Classif. (EU)	Reference
TNO-26 (Ink-3)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.1	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-27 (Thermal paper coating-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.6	9	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-28 (Toilet cleaner-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.4	0.8	12	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-29 (Toilet cleaner-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.3	1	11	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-30 (Pesticide-3)	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1.5	1	7	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-31 (Sulfur)	7704-34-9	solid	I	undiluted	n.p.	n.p.	-	0.2	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-32 (Ink-4)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	7	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-33 (Thermal paper coating-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2	0.5	5	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-34 (Detergent-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	1	25	1	1	I	I	R41	R41	Prinsen (1996)	
TNO-35 (Propyl-lactate)	616-09-1	liquid	S	undiluted	n.p.	n.p.	-	3	3	45	1	1	I	I	R41	R41	Prinsen (1996)	
TNO-36 (Ethylhexyl lactate)	6283-86-9	liquid	n.p.	undiluted	n.p.	n.p.	-	2	2	18	2A	2A	II	II	R36	R36	Prinsen (1996)	
TNO-37 (Pesticide-4)	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1.5	1	15	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-38 (Solvent-10)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-39 (Detergent-3)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.5	0.5	4	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-40 (Glycolbromoacetate form.)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2.6	1.9	41	1	1	I	I	R41	R41	Prinsen (1996)	
TNO-41 (Amidosulfonic acid)	5329-14-6	solid	n.p.	undiluted	n.p.	n.p.	-	2.7	4	46	1	1	I	I	R41	R41	Prinsen (1996)	
TNO-42 (Glycolbromoacetate)	3785-34-0	liquid	85%	n.p.	n.p.	n.p.	-	3	3	36	1	1	I	I	R41	R41	Prinsen (1996)	
TNO-43 (Monobromoacetic acid)	79-08-3	solid	S	undiluted	n.p.	n.p.	-	3	4	80	1	1	I	I	R41	R41	Prinsen (1996)	
TNO-44 (Didecyldimethylammoniumchloride (23% in propyl glycol))	7173-51-5	liquid	n.p.	23%	n.p.	n.p.	-	3	3.5	39	1	1	I	I	R41	R41	Prinsen (1996)	
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	2.0	2.0	22	1		I		R41		Prinsen (2000)	
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.8	1.7	21	1		I		R41		Prinsen (2000)	
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	2.0	2.0	21	1		I		R41		Prinsen (2000)	
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.7	1.7	18	1		I		R41		Prinsen (2000)	
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	1.8	2.5	14	2A		II		R36		Prinsen (2000)	
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	1.7	2.0	13	2A		II		R36		Prinsen (2000)	
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	2.0	2.3	17	2A		II		R36		Prinsen (2000)	
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	2.0	2.3	14	2A		II		R36		Prinsen (2000)	
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	2.0	2.0	13	2A		II		R36		Prinsen (2000)	
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.3	0.3	1	NI		NI		NI		Prinsen (2000)	
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.3	0.3	1	NI		NI		NI		Prinsen (2000)	
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.0	0.5	2	NI		NI		NI		Prinsen (2000)	
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.0	0.0	0	NI		NI		NI		Prinsen (2000)	
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.0	0.0	2	NI		NI		NI		Prinsen (2000)	

## *In Vitro* Data for Substances Tested in the ICE Test Method: Sorted by Reference

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	<i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	Overall <i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	<i>In Vitro</i> Classif. (EPA) <sup>3,4</sup>	Overall <i>In Vitro</i> Classif. (EPA)	<i>In Vitro</i> Classif. (EU) <sup>5,6</sup>	Overall <i>In Vitro</i> Classif. (EU)	Reference	
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	14	2B	2B	III	III	NI	NI	Prinsen (2000)	
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	14	2B		III		NI		Prinsen (2000)	
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	13	2B	III	III		NI	NI	Prinsen (2000)	
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.8	8	2B		III		NI		Prinsen (2000)	
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	11	2B	III	III		NI		Prinsen (2000)	
TNO-45	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	5	NI		NI	NI	NI	NI	NI	Prinsen (2005)
TNO-46	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-47	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-48	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	3	1	25	2A	2A	II	II	R36	R36	Prinsen (2005)	
TNO-49	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	3	4	-	1	1	I	I	R41	R41	Prinsen (2005)	
TNO-50	n.p.		n.p.	undiluted	n.p.	n.p.	-	3	3	41.1	1	1	I	I	R41	R41	Prinsen (2005)	
TNO-51	n.p.		n.p.	undiluted	n.p.	n.p.	-	3	3	33.9	1	1	I	I	R41	R41	Prinsen (2005)	
TNO-52	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.7	1	5	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-53	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.5	0.2	3	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-54	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1	1	9	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-55	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.7	1.3	10	2B	2B	III	III	R36	R36	Prinsen (2005)	
TNO-56	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2	1.3	10	2B	2B	III	III	R36	R36	Prinsen (2005)	
TNO-57	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.5	1.3	12	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-58	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	-1	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-59	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.2	0	-2	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-60	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0.5	1	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-61	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-62	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2	1	12	2B	2B	III	III	R36	R36	Prinsen (2005)	
TNO-63	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.3	0.5	3	NI	NI	IV	IV	NI	NI	NI	Prinsen (2005)
TNO-64	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	1	1	5	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-65	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	0.7	0.5	4	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-66	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-67	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	1	6	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-68	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1/2	1	8	2A	2A	II	II	R36	R36	Prinsen (2005)	
TNO-69	n.p.	liquid	n.p.	50%	n.p.	n.p.	-	1	0	0	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-70	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	2	1	20	2A	2A	II	II	R36	R36	Prinsen (2005)	
TNO-71	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	1	0.5	13	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-72	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	1.5	0.5	5	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-73	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	2.7	2	18	1	1	I	I	R41	R41	Prinsen (2005)	
TNO-74	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.5	0	0	NI	NI	IV	IV	NI	NI	NI	Prinsen (2005)
TNO-75	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	2	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-76	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	2	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-77	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	7	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-78	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.3	1	15	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-79	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1	1	10	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-80	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.3	0	-1	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-81	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-82	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0	0	-2	NI	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-83	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0.8	0.7	10	2B	2B	III	III	NI	NI	NI	Prinsen (2005)
TNO-84	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0.7	0.7	2	2B	2B	III	III	NI	NI	NI	Prinsen (2005)

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Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	<i>In Vitro</i> Classif. (GHS) <sup>1,2</sup>	Overall <i>In Vitro</i> Classif. (GHS)	<i>In Vitro</i> Classif. (EPA) <sup>3,4</sup>	Overall <i>In Vitro</i> Classif. (EPA)	<i>In Vitro</i> Classif. (EU) <sup>5,6</sup>	Overall <i>In Vitro</i> Classif. (EU)	Reference
TNO-85	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	2	1.3	14	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-86	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	1	1	7	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-87	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.7	1	1	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-88	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.3	0.7	3	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-89	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.2	0.7	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-90	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-91	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0.2	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-92	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.8	1.7	16	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-93	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	3	2	17	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-94	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
1-Butanol	71-36-3	liquid	S	undiluted	99%	Aldrich	-	2.9	2	54	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
2-Butoxyethyl acetate	112-07-2	liquid	S	undiluted	99%	Aldrich	-	1	1	5	2B	2B	III	III	NI	NI	Prinsen and Koëter (1993)
2-Methoxyethanol	109-86-4	liquid	S	undiluted	99.9%	Aldrich	-	2	2	18	2A	2A	II	II	R36	R36	Prinsen and Koëter (1993)
Acetaldehyde	75-07-0	liquid	S	undiluted	99%	Aldrich	-	2	1.4	24	2A	2A	II	II	R36	R36	Prinsen and Koëter (1993)
Acetic acid	64-19-7	liquid	S	10%	99%	Aldrich	-	3	2.6	31	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
Benzalkonium chloride (100%)	8001-54-5	liquid	S	undiluted	n.p.	Aldrich	-	3	3	40	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
Brij 35	9002-92-0	liquid	S	undiluted	n.p.	Aldrich	-	0.9	0	5	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Chloroform	67-66-3	liquid	I*	undiluted	99.8%	Aldrich	-	2.5	1	21	2A	2A	II	II	R36	R36	Prinsen and Koëter (1993)
Dibutyltin dichloride	683-18-1	solid	S	undiluted	97%	Aldrich	-	3	2.5	34	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
Dimethyl sulfoxide	67-68-5	liquid	S	undiluted	99.9%	Aldrich	-	1	0.5	4	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Glycerol	56-81-5	liquid	S	undiluted	99%	Aldrich	-	0.5	0.4	4	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Mercury (II) chloride	7487-94-7	solid	I	undiluted	99.5%	Aldrich	-	2	3.1	55	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
n-Hexane	110-54-3	liquid	I	undiluted	99%	Aldrich	-	0.5	0	1	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Silver (I) nitrate	7761-88-8	solid	S	3%	99.5%	Aldrich	-	1	1	12	2B	2B	III	III	NI	NI	Prinsen and Koëter (1993)
Sodium dodecyl sulfate	151-21-3	solid	S	undiluted	70%	Aldrich	-	0.8	1	22	2B	2B	III	III	R41	R41	Prinsen and Koëter (1993)
Sodium fluorescein	518-47-8	liquid	S	20%	70% <sup>8</sup>	Aldrich	-	0.1	0	0	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Sodium hydroxide	1310-73-2	liquid	S	1%	97%	Aldrich	-	3	3	60	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
Toluene	108-88-3	liquid	I*	undiluted	99.9%	Aldrich	-	1.1	1.4	4	2B	2B	III	III	NI	NI	Prinsen and Koëter (1993)
Triaacetin	102-76-1	liquid	I*	undiluted	99%	Aldrich	-	0.5	0.4	4	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Tributyltin chloride	1461-22-9	liquid	n.p.	undiluted	96%	Aldrich	-	3	2.5	48	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
Triethanolamine	102-71-6	liquid	S	undiluted	99%	Aldrich	-	0.9	0.7	4	2B	2B	III	III	NI	NI	Prinsen and Koëter (1993)

Abbreviations: S = soluble; SF = surfactant; I = insoluble; \*solubility uncertain; RG = reagent grade; n.p. = not provided and not obtained

<sup>1</sup>GHS=Globally Harmonized System (UN 2007)

<sup>2</sup>Eve Irritant Category 1 = irreversible effects on the eve/serious damage to the eve; Category 2A = reversible effects on the eve/irritating to the eyes; Category 2B = reversible effects on the eve/mildly irritating to the eyes; Nonirritant = not an eve irritant.

<sup>3</sup>FPA=U.S. Environmental Protection Agency (FPA 2003a)

<sup>4</sup>Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 1-7 days; Category IV: minimal effects clearing in less than 24 hr.

<sup>5</sup>EU=European Union (EU 2001).

<sup>6</sup>Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

<sup>7</sup>Numbering for substances from this reference assigned based on order of appearance in Table 3 of Prinsen (1996)

<sup>8</sup>Dye content